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ON THE TERMINAL WIENER INDEX OF THORN GRAPHS

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ABSTRACT. The *terminal Wiener index* $TW = TW(G)$ of a graph G is equal to the sum of distances between all pairs of pendent vertices of G. This distance–based molecular structure descriptor was put forward quite recently [I. Gutman, B. Furtula, M. Petrović, *J. Math. Chem.* **46** (2009) 522–531]. In this paper we report results on TW of thorn graphs. Also a method for calculation of TW of dendrimers is described.

INTRODUCTION

Let G be a connected graph with vertex set $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $\mathbf{E}(G) = \{e_1, e_2, \ldots, e_m\}$. The *distance* between the vertices v_i and v_j, $v_i, v_j \in \mathbf{V}(G)$, is equal to the length (= number of edges) of the shortest path starting at v_i and ending at v_j (or vice versa) [1], and will be denoted by $d(v_i, v_j|G)$.

The oldest molecular structure descriptor (topological index) is the one put forward in 1947 by Harold Wiener [2], nowadays referred to as the *Wiener index* and denoted by W. It is defined as the sum of distances between all pairs of vertices of a (molecular) graph:

$$W = W(G) = \sum_{\{u,v\} \subseteq \mathbf{V}(G)} d(u,v|G) = \sum_{1 \leq i < j \leq n} d(v_i,v_j|G) \ . \tag{1}$$

Details on the chemical applications and mathematical properties of the Wiener index can be found in the reviews [3–5].

The square matrix of order n whose (i,j)-entry is $d(v_i,v_j|G)$ is called the *distance matrix* of G. Also this matrix has been much studied by mathematical chemists, for details see [6, 7]. From the distance matrix not only the Wiener index, but also numerous other structure descriptors can be derived [8, 9].

In a number of recently published articles, the so-called *terminal distance matrix* [10, 11] or *reduced distance matrix* [12] of trees was considered.

If an n-vertex graph G has k pendent vertices (= vertices of degree one), labeled by $v_1, v_2, \ldots, v_k$, then its terminal distance matrix is the square matrix of order k whose (i,j)-entry is $d(v_i,v_j|G)$.

Terminal distance matrices were used for modeling of amino acid sequences of proteins and of the genetic code [10, 11, 13], and were proposed to serve as a source of novel molecular–structure descriptors [10, 11].

Motivated by the previous researches on the terminal distance matrix and on its chemical applications, the present authors have conceived the *terminal Wiener index* $TW(G)$ of a graph G as *the sum of the distances between all pairs of its pendent vertices* [14].

Without loss of generality, we may assume that the graph G has n vertices of which k vertices, labeled by $v_1, v_2, \ldots, v_k$, are pendent. Let thus $\mathbf{V}_1(G) = \{v_1, v_2, \ldots, v_k\}$ be the set of pendent vertices of G. In harmony with the previously introduced notation, $\mathbf{V}_1(G) \subseteq \mathbf{V}(G)$. Then, in analogy with Eq. (1), we define

$$TW = TW(G) = \sum_{\{u,v\} \subseteq \mathbf{V}_1(G)} d(u,v|G) = \sum_{1 \leq i < j \leq k} d(v_i,v_j|G) \ . \tag{2}$$

In addition to [14], there seems to exist only one more paper [15] on terminal Wiener index. Thus, neither the theory nor the chemical applications of TW are nowadays well elaborated. The aim of the present work is to contribute towards filling this gap.

TERMINAL WIENER INDEX OF THORN GRAPHS

Let G a connected n-vertex graph with vertex set $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$, and let $\mathbf{p} = (p_1, p_2, \ldots, p_n)$ be an n-tuple of non-negative integers. The *thorn graph* $G_\mathbf{p}$ is the graph obtained by attaching p_i pendent vertices to the vertex v_i of G for $i = 1, 2, \ldots, n$. The p_i pendent vertices attached to the vertex v_i will be called the thorns of v_i.

The concept of thorny graphs was introduced by one of the present authors [16], and eventually found a variety of chemical applications [17–22]. We now show how, in the general case, one can compute the terminal Wiener index of a thorn graph.

Theorem 1. Let $G_\mathbf{p}$ be the thorn graph, obtained by attaching p_i terminal vertices to the vertex v_i of the connected graph G, $i = 1, 2, \ldots, n$. If $p_i > 0$ for all $i = 1, 2, \ldots, n$, then

$$TW(G_\mathbf{p}) = 2 \sum_{i=1}^{n} \binom{p_i}{2} + \sum_{1 \leq i < j \leq n} p_i \, p_j \, [d(v_i, v_j|G) + 2] \, . \tag{3}$$

Proof. We obtain formula (3) by applying Eq. (2). Consider first the thorns attached to a given vertex v_i. Each of these are at distance 2, and therefore their contribution to $TW(G_\mathbf{p})$ is $\binom{p_i}{2} \times 2$. This leads to the first term on the right–hand side of (3).

Consider a thorn attached to vertex v_i and a thorn attached to vertex v_j, $i \neq j$. Their distance is by two greater than the distance between v_i and v_j. Since there are $p_i \times p_j$ pairs of thorns of this kind, their contribution to $TW(G_\mathbf{p})$ is equal to $p_i \, p_j \, [d(v_i, v_j|G) + 2]$. This leads to the second term on the right–hand side of (3). ■

Corollary 1.1. Formula (3) remains valid also if some p_i's are equal to zero, provided that the corresponding vertices of the graph G are not pendent.

Corollary 1.2. If $p_1 = p_2 = \cdots = p_n = p > 0$, then

$$TW(G_\mathbf{p}) = p^2 \, W(G) + pn(pn - 1) \, . \tag{4}$$

Proof. Start with Eq. (3) and apply the definition (1) of the Wiener index of the graph G. This yields

$$TW(G_{\mathbf{p}}) = np(p-1) + p^2\ [W(G) - n(n-1)]$$

which is then easily transformed into Eq. (4). ∎

Corollary 1.3. Let the graph G be not connected, and consist of a (connected) component G^* and some other components. Let all pendent vertices of G (if any) belong to G^*. Let $\mathbf{V}(G^*) = \{v_1, v_2, \ldots, v_{n^*}\}$. If all thorns of $G_{\mathbf{p}}$ are on vertices of G^*, and if each vertex of G^* possesses at least one thorn, then

$$TW(G_{\mathbf{p}}) = 2\sum_{i=1}^{n^*} \binom{p_i}{2} + \sum_{1 \le i < j \le n^*} p_i\, p_j\, [d(v_i, v_j | G^*) + 2]\ .$$

Corollary 1.4. If the conditions specified in Corollary 1.3 hold, and if $p_1 = p_2 = \cdots = p_{n^*} = p > 0$, then

$$TW(G_{\mathbf{p}}) = p^2\, W(G^*) + p\, n^*\, (p\, n^* - 1)\ .$$

Theorem 2. Let G be a connected n-vertex graph, and let $v_1, v_2, \ldots, v_k$ be its pendent vertices. Choose the n-tuple $\mathbf{p}$ so that

$$p_i = \begin{cases} p & \text{for } i = 1, 2, \ldots, k \\ 0 & \text{for } i = k+1, \ldots, n \end{cases}$$

and let $p > 0$. Then

$$TW(G_{\mathbf{p}}) = p^2\, TW(G) + pk(pk-1)\ . \tag{5}$$

Proof. Start with Eq. (3) and apply the definition (2) of the terminal Wiener index of the graph G. This yields

$$TW(G_{\mathbf{p}}) = kp(p-1) + p^2\ [TW(G) - k(k-1)]$$

which is then easily transformed into Eq. (5). ∎

Note that if in the above theorem $p = 0$, then $TW(G_{\mathbf{p}}) \equiv TW(G)$.

Note also that Eq. (5) is a kind of recurrence relation, because the terminal Wiener index of a bigger graph (namely of $G_{\mathbf{p}}$) is expressed in terms of the terminal Wiener index of a smaller graph (namely of G). This observation will be utilized in the subsequent section.

APPLICATION TO DENDRIMERS

By means of Theorem 2 it is possible to recursively compute the terminal Wiener indices of certain dendrimers. An example of a dendrimer series to which formula (5) is applicable is shown in Fig. 1.

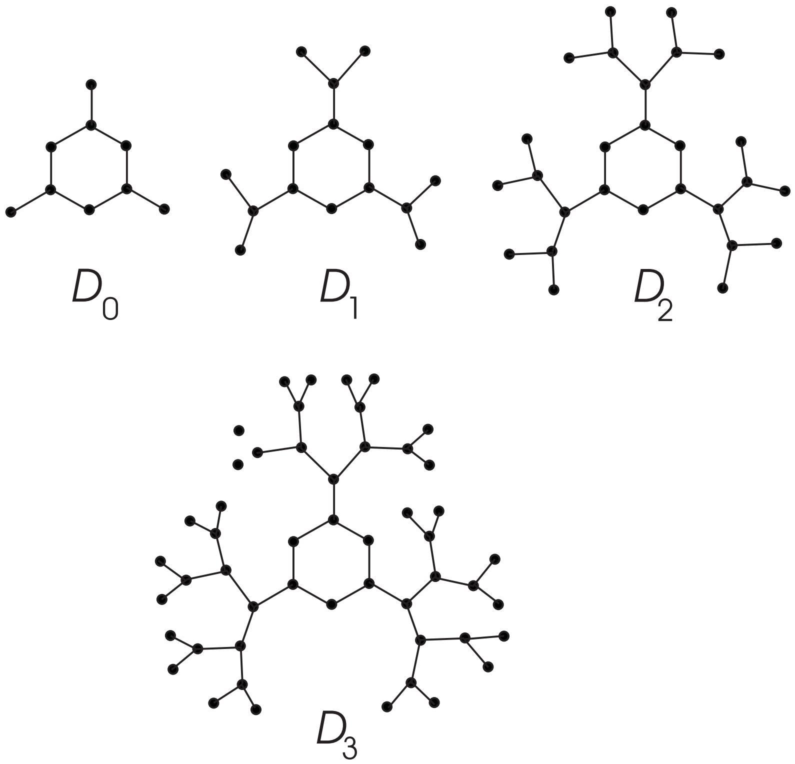

Fig. 1. The first four members of a series of dendrimer graphs. Their terminal Wiener indices are calculated recursively as $TW(D_0) = 12$, $TW(D_1) = 78$, $TW(D_2) = 444$, $TW(D_3) = 2328$, ...; for details see text.

Let D_0, D_1, D_2, ... be a series of dendrimer graphs. Let for $h = 1, 2, \ldots$, the dendrimer graph D_h be obtained so that p pendent vertices are attached to each pendent vertex of D_{h-1}. For an illustration see Fig. 1.

Details on dendrimers, an important and recently much studied class of nano-materials, and especially on their topological properties can be found in the books [23, 24] and the references quoted therein.

Let k_h be the number of pendent vertices of D_h. Then from Theorem 2 we get the recurrence relations:

$$\begin{aligned} TW(D_{h+1}) &= p^2\, TW(D_h) + p\, k_h (p\, k_h - 1) \\ k_{h+1} &= p\, k_h \ . \end{aligned}$$

In the examples depicted in Fig. 1, $p = 2$. It is easy to check that $TW(D_0) = 12$ and $k_0 = 3$. Then

$$\begin{aligned} TW(D_1) &= p^2\, TW(D_0) + p\, k_0 (p\, k_0 - 1) = 2^2 \cdot 12 + 2 \cdot 3 \cdot (2 \cdot 3 - 1) = 78 \\ k_1 &= p\, k_0 = 2 \cdot 3 = 6 \end{aligned}$$

$$\begin{aligned} TW(D_2) &= p^2\, TW(D_1) + p\, k_1 (p\, k_1 - 1) = 2^2 \cdot 78 + 2 \cdot 6 \cdot (2 \cdot 6 - 1) = 444 \\ k_2 &= p\, k_1 = 2 \cdot 6 = 12 \end{aligned}$$

$$\begin{aligned} TW(D_3) &= p^2\, TW(D_2) + p\, k_2 (p\, k_2 - 1) = 2^2 \cdot 444 + 2 \cdot 12 \cdot (2 \cdot 12 - 1) = 2328 \\ k_3 &= p\, k_2 = 2 \cdot 12 = 24 \end{aligned}$$

$$\begin{aligned} TW(D_4) &= p^2\, TW(D_3) + p\, k_3 (p\, k_3 - 1) = 2^2 \cdot 2328 + 2 \cdot 24 \cdot (2 \cdot 24 - 1) = 11568 \\ k_4 &= p\, k_3 = 2 \cdot 24 = 48 \end{aligned}$$

etc.

CONCLUDING REMARKS

As already mentioned, the terminal Wiener index is a very new molecular–structure descriptor. Only a limited number of its mathematical properties were established so far [14, 15].

Until now no attempt was reported to find some chemical application of TW or, at least, to investigate how TW is correlated with the usually employed physico–chemical properties of alkanes (octane isomers, in particular). The same applies to the TW-values of dendrimers. It remains a task for the future to work along these lines.

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